Benzenesulfonic acid, 3-hydrazino-138-30-7 | DTXSID8059681

Model Performance

Weighted KNN model

| 5-fold CV (75%) | | Training (| Training (75%) | | Test (25%) | |
|-----------------|------|------------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 | |

Model Results

Predicted value: 3.29 days

Global applicability domain: Inside

Local applicability domain index: 5.10e-01

Confidence level: 9.19e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5 Predicted: 3.17

Image not found

3-Ethyltoluene

Measured: 12.5 Predicted: 3.26

Image not found

1-Ethyl-2-methylbenzene

Measured: 24.3 Predicted: 3.88

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 24.3 Predicted: 3.89

Image not found

2-Ethyl-p-xylene Measured: 12.5 Predicted: 3.70